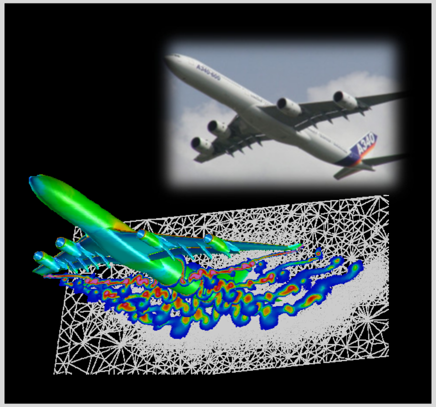

High Performance Computing

ADVANCED SCIENTIFIC COMPUTING

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LECTURE 4

Advanced MPI Techniques

September 19, 2019

Room V02-258

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

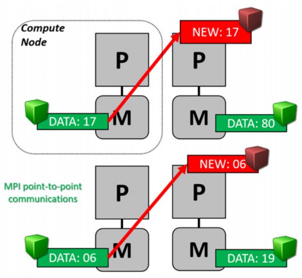
DEEP Projects

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

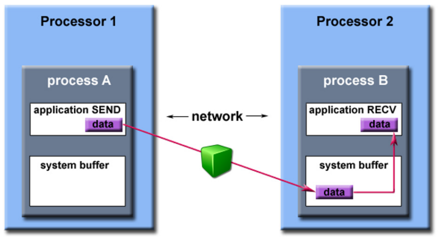
HAICU HELMHOLTZ ARTIFICIAL INTELLIGENCE COOPERATION UNIT

Review of Practical Lecture 3.1 – Understanding MPI Messages & Collectives

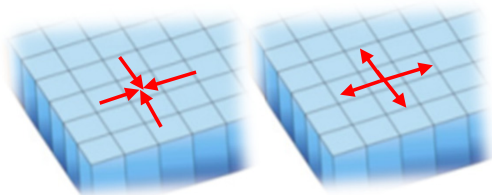
- MPI purpose: send data as messages to other processors



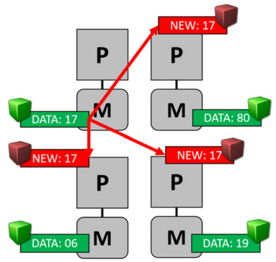
MPI
Point
to
Point
Communication

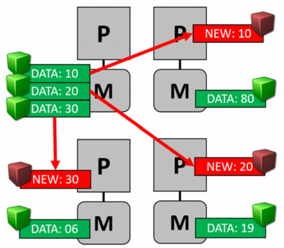



```
MPI_Init(&argc, &argv);

MPI_Comm_size(MPI_COMM_WORLD, &numtasks);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);

if (rank == 0) {
  dest = 1; source = 1;
  rc = MPI_Send(&outmsg, 1, MPI_CHAR, dest, tag, MPI_COMM_WORLD);
  rc = MPI_Recv(&inmsg, 1, MPI_CHAR, source, tag, MPI_COMM_WORLD, &Stat);
}
else if (rank ==1 ) {
  dest = 0; source = 0;
  rc = MPI_Recv(&inmsg, 1, MPI_CHAR, source, tag, MPI_COMM_WORLD, &Stat);
  rc = MPI_Send(&outmsg, 1, MPI_CHAR, dest, tag, MPI_COMM_WORLD);
}

rc = MPI_Get_count(&Stat, MPI_CHAR, &count);
```



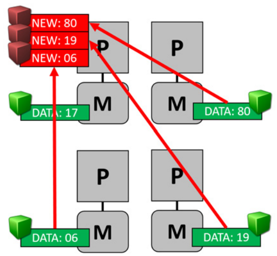
(e.g. using MPI messages in scientific simulations)

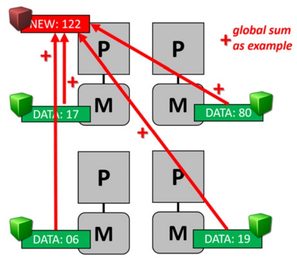




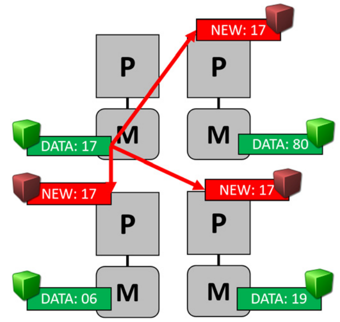
MPI
Collective
Communication

[1] LLNL MPI Tutorial






```
MPI_Init(&argc,&argv);

MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
MPI_Comm_rank(MPI_COMM_WORLD,&rank);

source=0;
count=4;

if(rank == source){
  for(i=0;i<count;i++)
    buffer[i]=i;
}

MPI_Bcast(buffer,count,MPI_INT,source,MPI_COMM_WORLD);

for(i=0;i<count;i++)
  printf("%d \n",buffer[i]);

MPI_Finalize();
```



(e.g. instead of using a for loop & MPI_Send/Recv multiple times)

Outline of the Course

1. High Performance Computing
2. Parallel Programming with MPI
3. Parallelization Fundamentals
4. Advanced MPI Techniques
5. Parallel Algorithms & Data Structures
6. Parallel Programming with OpenMP
7. Graphical Processing Units (GPUs)
8. Parallel & Scalable Machine & Deep Learning
9. Debugging & Profiling & Performance Toolsets
10. Hybrid Programming & Patterns
11. Scientific Visualization & Scalable Infrastructures
12. Terrestrial Systems & Climate
13. Systems Biology & Bioinformatics
14. Molecular Systems & Libraries
15. Computational Fluid Dynamics & Finite Elements
16. Epilogue

+ additional practical lectures & Webinars for our hands-on assignments in context

- Practical Topics
- Theoretical / Conceptual Topics

Outline

- Advanced MPI Communication Techniques
  - Blocking vs. Non-Blocking Communication
  - MPI Communicators & Creating Sub-Groups
  - MPI Cartesian Communicator & Application Motivations
  - Hardware & Communication Issues & Network Interconnects
  - Task-Core Mappings & Heatmap Application Example

- MPI Parallel I/O Techniques
  - I/O Terminologies & Challenges
  - Parallel Filesystems & Striping Technique
  - MPI I/O Techniques & Use of Parallel I/O
  - Higher-Level I/O Libraries & Community Standards
  - Portable File Formats & Data Science Application Example

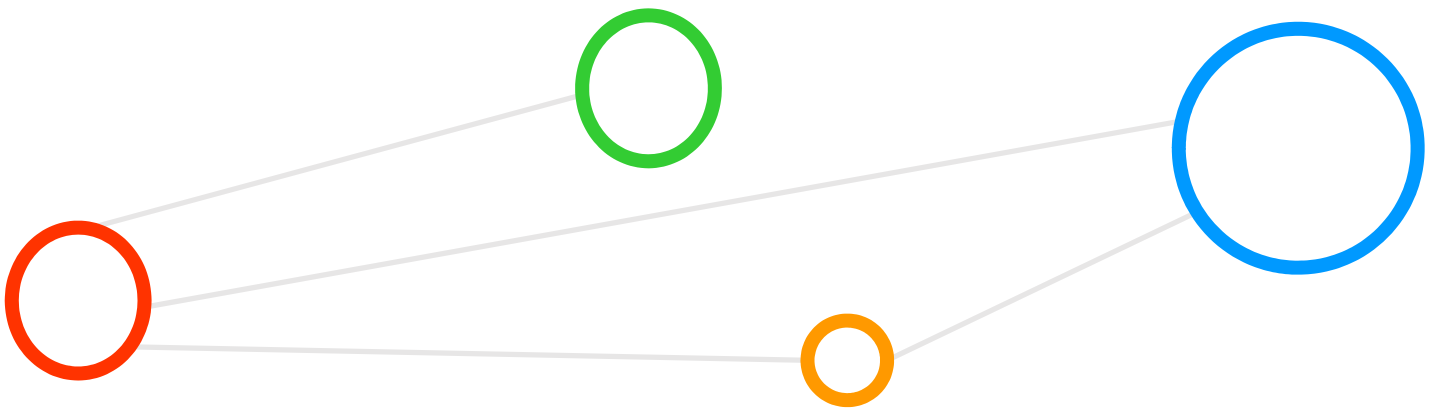
- **Promises from previous lecture(s):**
- ***Lecture 1:*** **Lecture 2 & 4 will give in-depth details on the distributed-memory programming model with the Message Passing Interface (MPI)**
- ***Lecture 2:*** **Lecture 4 will provide more details on advanced functions of the Message Passing Interface (MPI) standard & its use in applications**
- ***Lecture 2:*** **Lecture 4 on advanded MPI techniques will provide details about the often used MPI cartesian communicator & its use in applications**
- ***Practical Lecture 3.1:*** **Lecture 4 will offer more insights about using different types of MPI communicators with different rank identities in MPI applications**
- ***Practical Lecture 3.1:*** **Lecture 4 will offer more insights about using blocking communication vs. non-blocking communication functions when using MPI**
- ***Practical Lecture 3.1:*** **Lecture 4 will offer more insights about using the MPI status for different purposes and to obtain a better understanding what happens**

Selected Learning Outcomes

- Students understand…
  - Latest developments in parallel processing & high performance computing (HPC)
  - How to create and use high-performance clusters
  - What are scalable networks & data-intensive workloads
  - The importance of domain decomposition
  - Complex aspects of parallel programming
  - HPC environment tools that support programming or analyze behaviour
  - Different abstractions of parallel computing on various levels
  - Foundations and approaches of scientific domain-specific applications

- Students are able to …
  - Programm and use HPC programming paradigms
  - Take advantage of innovative scientific computing simulations & technology
  - Work with technologies and tools to handle parallelism complexity

Advanced MPI Communication Techniques

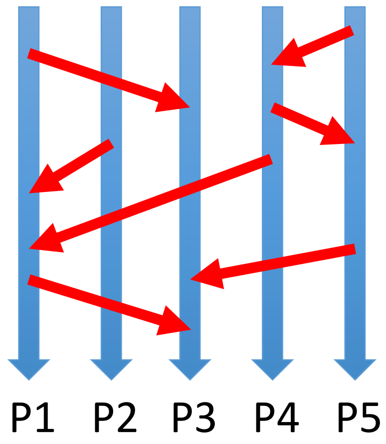


Programming with Distributed Memory using MPI – Revisited (cf. Lecture 1)

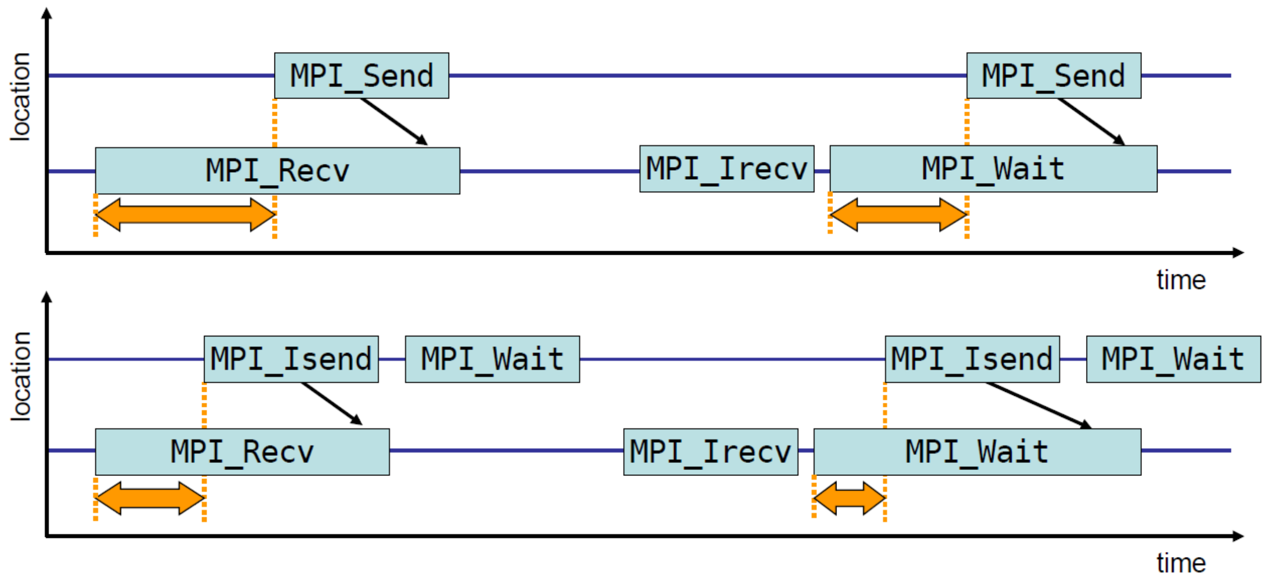
- **Distributed-memory programming enables explicit message passing as communication between processors**
- **Message Passing Interface (MPI) is dominant distributed-memory programming standard today (available in many different version)**
- **MPI is a standard defined and developed by the MPI Forum**

[4] MPI Standard

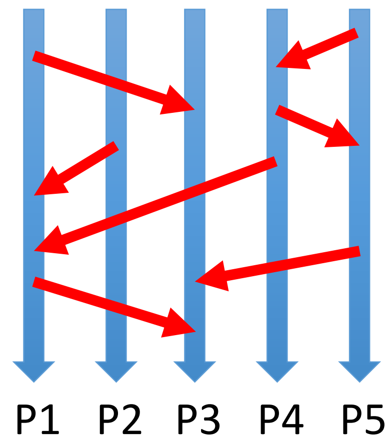
- Features
  - No remote memory access on distributed-memory systems
  - Require to ‘send messages’ back and forth between processes PX
  - Many free Message Passing Interface (MPI) libraries available
  - Programming is tedious & complicated, but most flexible method



Blocking vs. Non-blocking communication



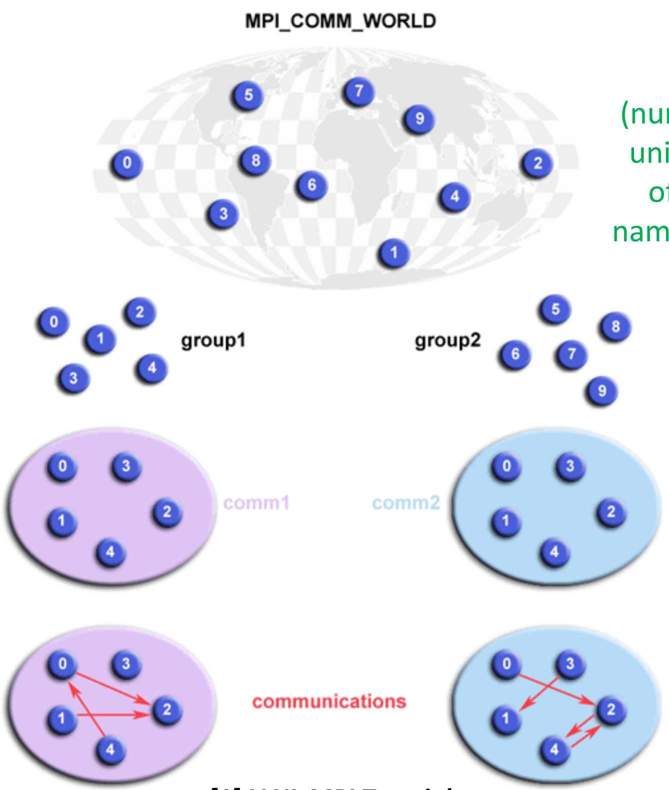
[5] Metrics tour



- **Blocking vs. non-blocking: MPI_Send() blocks until data is received; MPI_Isend() continues**
- **The use of these functions can cause different performance problems (e.g. here 'late sender')**
- **MPI_Wait() does wait for a given MPI request to complete before continuing**
- **MPI_Waitall() does wait for all given MPI requests (e.g. waiting for message) to complete before continuing**

➢ **Lecture 5 offers more details on using blocking & non-blocking MPI communication in simulations and data science applications**

Using MPI Ranks & Communicators – Revisited (cf. Lecture 2)



(numbers reflect unique identity of processor named 'MPI rank)

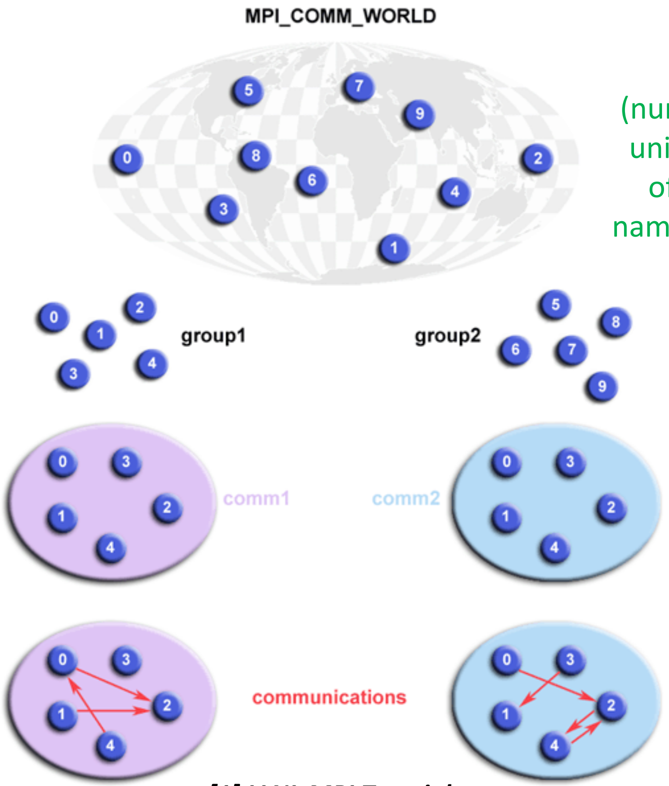
[1] LLNL MPI Tutorial

- Answers the following question:
  - How do I know where to send/receive to/from?
- Each MPI activity specifies the context in which a corresponding function is performed
  - MPI_COMM_WORLD (region/context of all processes)
  - Create (sub-)groups of the processes / virtual groups of processes
  - Peform communications only within these sub-groups easily with well-defined processes

- **Using communicators wisely in collective functions can reduce the number of affected processors**
- **MPI rank is a unique number for each processor**

MPI Communicators – MPI Create Sub-Group Communicators

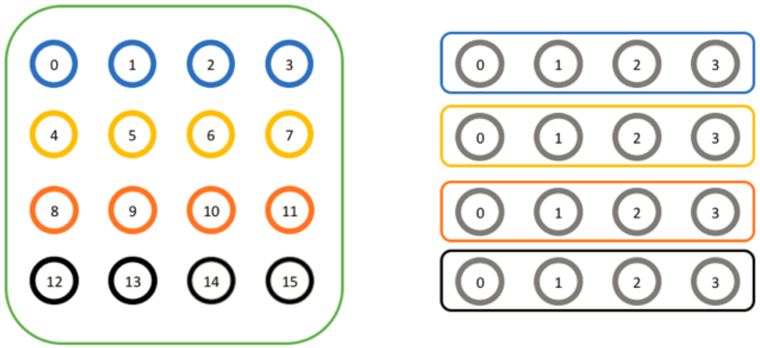
- Create (sub-)groups of the processes & virtual groups of processes
  - Simple to complex communicator setups
  - E.g. split existing communicator using `MPI_Comm_split()`
  - Free new communictors: `MPI_Comm_free()`



[1] LLNL MPI Tutorial

(numbers reflect unique identity of processor named 'MPI rank)

- **MPI_Comm_split() creates a new smaller communicator out of a larger communicator by splitting its current ranks (e.g., rows)**
- **New rank identities are created in the newly created communicator**
- **MPI ranks in different communicators represent different unique identifiers**



[2] Introduction to Groups & Communicators

Using MPI_Comm_split() & MPI_Comm_free() – Row Communicator Example

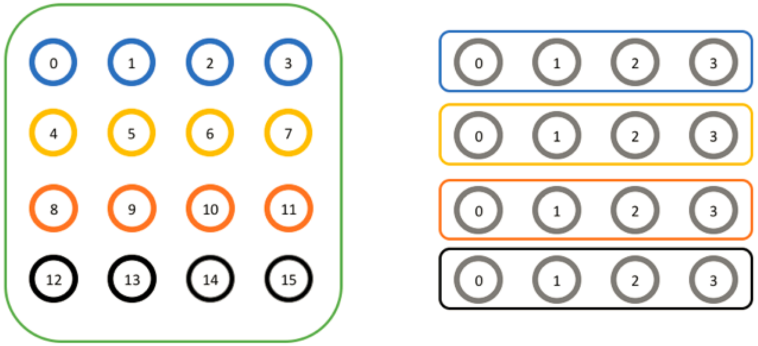
```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char** argv) {
  int world_rank, world_size;
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &world_size);
  MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);
  int color = world_rank / 4;
  MPI_Comm row_comm;
  MPI_Comm_split(MPI_COMM_WORLD, color, world_rank, &row_comm);
  int row_rank, row_size;
  MPI_Comm_size(row_comm, &row_size);
  MPI_Comm_rank(row_comm, &row_rank);
  printf("WORLD RANK/SIZE: %d/%d \t ROW RANK/SIZE: %d/%d\n",
         world_rank, world_size, row_rank, row_size);
  MPI_Comm_free(&row_comm);
  MPI_Finalize();
  return 0;
}
```

- **MPI_COMM_WORLD with all processors (cf. Lecture 2)**
- **Splitting scheme according to illustration matching colors / rows**

- **Definition of a new communicator and a split of the existing MPI_COMM_WORLD communicator using the defined row scheme via the function MPI_Comm_split()**

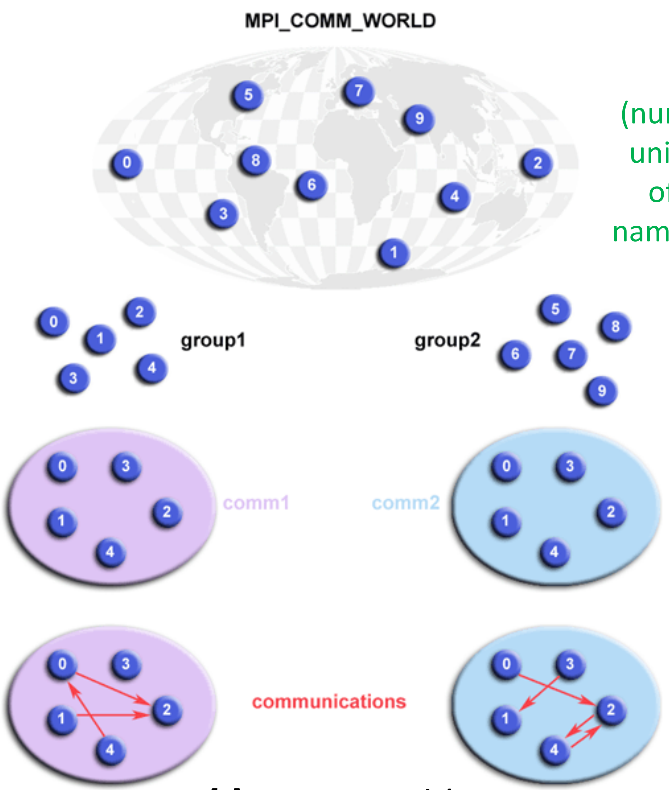
- **Different ranks and sizes for the newly created row communicator**
- **Print different identities in both communicators shows differences**

- **Free communicator**



[2] Introduction to Groups & Communicators

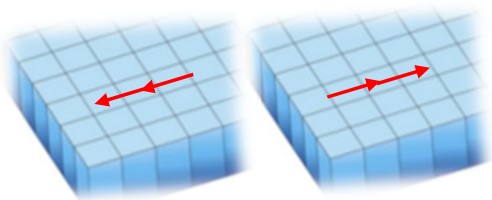
MPI Communicators – Create MPI Cartesian Communicators



[1] LLNL MPI Tutorial

(numbers reflect unique identity of processor named 'MPI rank)

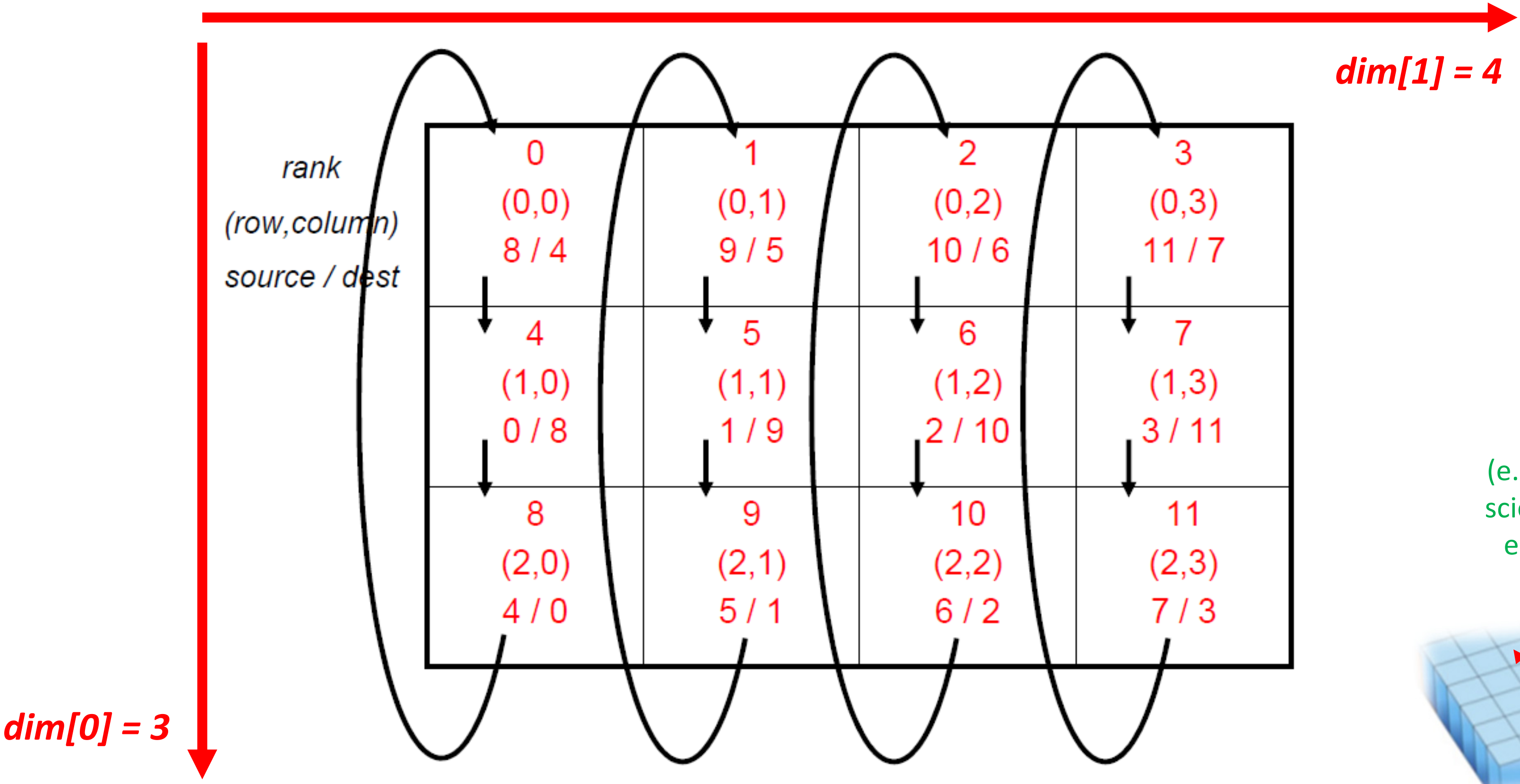
- Create (sub-)groups of the processes & virtual groups of processes
  - E.g. optimized for cartesian topology `MPI_Cart_create()`
  - Creates a new communicator out of MPI_COMM_WORLD
  - Dims: array with length for each dimension
  - Periods: logical array specifying whether the grid is periodic or not
  - Reorder: Allow reordering of ranks in output communicator



(e.g. using MPI messages in scientific simulations and/or engineering applications)

> ➢ **Assignment #3 will make use of the cartesian communicator in a simple application example that includes the moving of boats & fish**

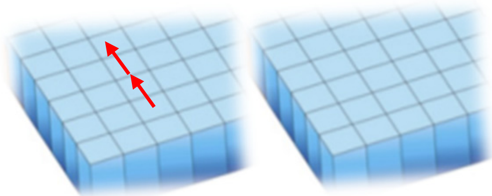
Cartesian Communicator Example – Conceptual View



('cartesian structure')

modified from [3] German MPI Lecture

(e.g. using MPI messages in scientific simulations and/or engineering applications)



Cartesian Communicator Example – Source-code View

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char** argv) {
  int rank, size;
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  dims[0]=3; dims[1] = 4;
  periods[0]=true; periods[1]=true;
  reorder = false;
  MPI_Cart_create(MPI_COMM_WORLD, 2, dims,
            periods, reorder, &comm_2d);
  MPI_Cart_coords(comm_2d, rank, 2, &coords);
  MPI_Cart_shift(comm_2d, 0, 1, &source, &dest);
  a = rank; b = 1;
  MPI_Sendrecv(a, 1, MPI_REAL, dest, 13, b, 1,
            MPI_REAL, source, 13, comm_2d, &status);
  MPI_Finalize();
  return 0;
}
```

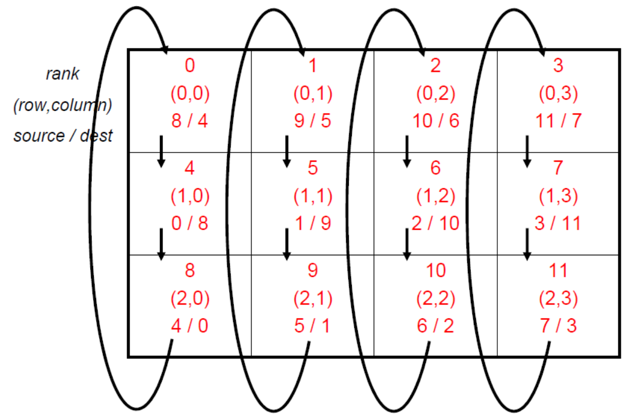
- **Preparing parameter dims as array with length for each dimension (here 3 x 4)**
- **Preparing parameter periods as logical array specifying whether the cartesian grid is period**
- **Preparing parameter reorder as not reordering of ranks in output communicator**

- **MPI_Cart_create() creates a new communicator (cartesian structure) according to specified dimensions in variables**

- **MPI_Cart_coords() obtains process coordinates in cartesian topology – note that this JUST obtaines the current process coordinates – no actual shift is done yet**
- **MPI_Cart_shift() obtains 'ranks' for shifting data in cartesian topology – note that this JUST prepares for a shift understanding which ranks are affected by shift**

- **A real shift is done using a typical MPI message exchange with the obtained ranks and in the space of the Cartesian communicator**

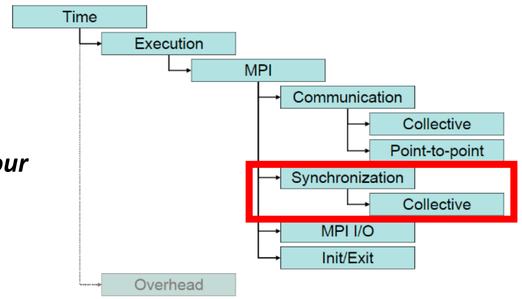
modified from [3] German MPI Lecture



Hardware & Communication Issues

- **Communication overhead can have significant impact on application performance**
- **Characteristics of interconnects of compute nodes/cpus affect parallel performance**

- Parallel Programming can cause communication issues
  - E.g. need for synchronisation in applications, e.g use of `MPI_Barriers()`
- Wide varieties of networks in HPC systems are available
  - Different network topologies of different types of networks used in HPC
- Gigabit Ethernet
  - Simple/cheep and good for high throughput computing (HTC)
  - Often too slow for parallel programs that require fast interconnects
- Infiniband
  - Fast, thus dominant distributed-memory computing interconnect today
  - Other interconnects exist but still less used: Intel Omnipath, Extoll, etc.



[5] Metrics tour

Communication Issues – Synchronisation with MPI Barrier Example

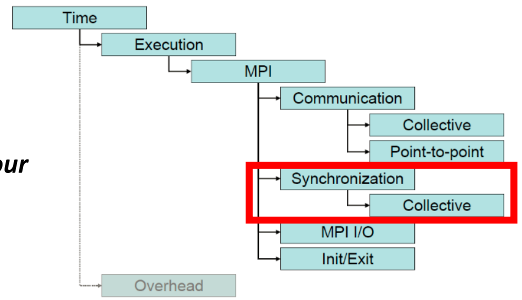
```
#include <stdio.h>
#include <mpi.h>
#include <unistd.h>
int main (int argc, char** argv) {
  int rank, size;
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  if (rank == 0) {
    sleep(10);
  }
  if (rank == 1) {
    storeResultsToFile();
  }
  MPI_Barrier(MPI_COMM_WORLD);
  MPI_Finalize();
  return 0;
}
```

- **One reason to require a synchronisation across processors is that one rank is performing some extraordinary long work, not others (e.g., master/worker parallelization technique, cf. Lecture 2)**
- **Sleep() is a function that puts a processor to sleep and thus doing basically nothing. Still a parallel computing resource is not usable for other users since it is typically exclusively allocated to one user by a scheduling system**

- **Another reason to require a synchronisation across processors is that one rank performs I/O operations of some kind (e.g., later in this lecture w/o using parallel I/O)**

- **MPI_Barrier() blocks the caller until all processes in the communicator have called it for synchronisation**

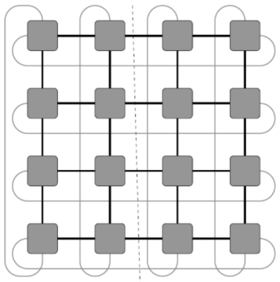
[5] Metrics tour

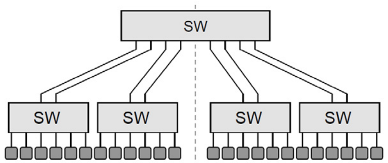


➢ **Lecture 9 on debugging, profiling & performance toolsets offers insights into performance analysis tools to understand MPI code better**

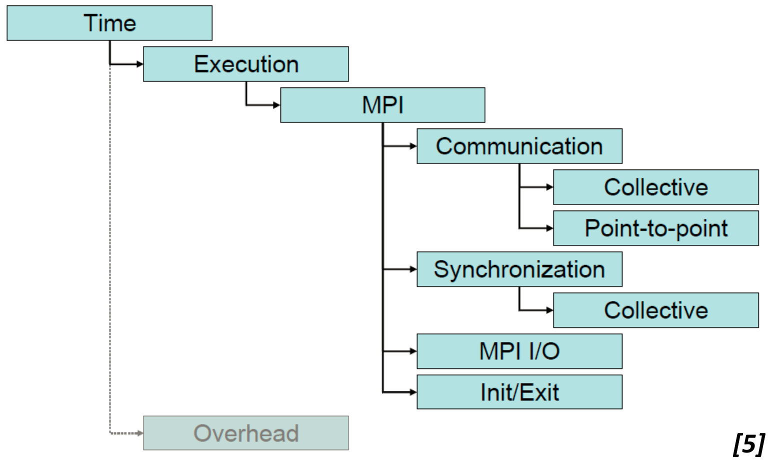
Optimization & Dependencies on Hardware & I/O

- Optimizations in terms of software & hardware are important
  - Optimization can be interpreted as using ‘dedicated‘ hardware features (if available)
  - E.g. network interconnections enable different used ‘network topologies‘ (varies in different systems)
  - E.g. parallel codes are tuned applying parallel I/O with parallel filesystems (if parallel filesystem exists)





[6] Introduction to High Performance Computing for Scientists and Engineers

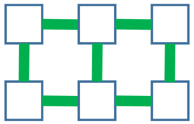


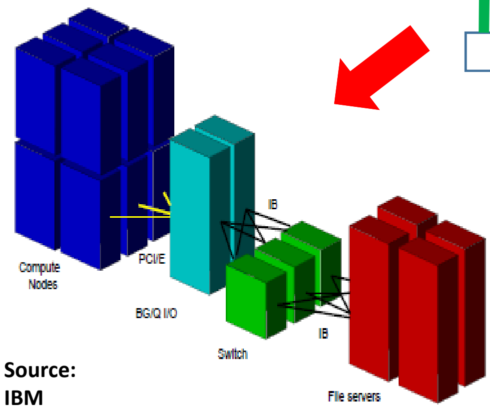
[5] Metrics tour

> **Lecture 9 on debugging, profiling & performance toolsets offers insights into performance analysis tools to understand MPI code better**

Complex Network Topologies & Challenges

- Large-scale HPC Systems have special network setups
  - Dedicated I/O nodes, fast interconnects, e.g. Infiniband (IB), Extoll, etc.
  - Different network topologies, e.g. tree, 5D Torus network, mesh, etc.
    (raise challenges in task mappings and communication patterns)





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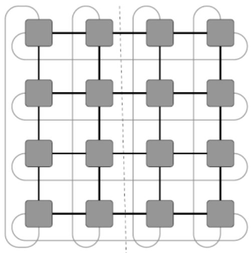
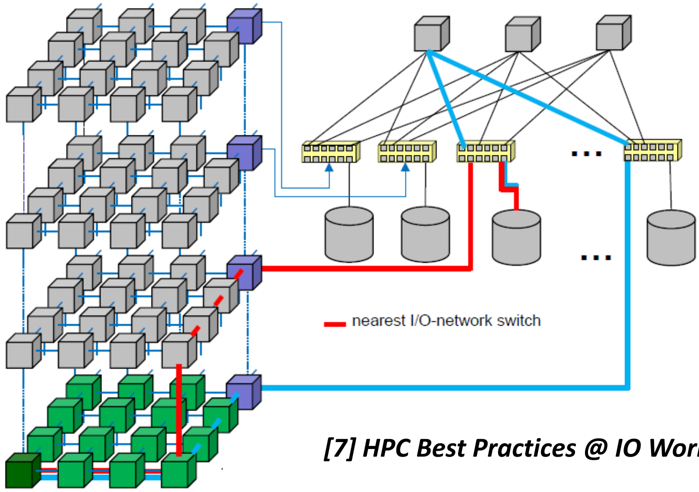


Contention and cross traffic caused by multiple I/O streams

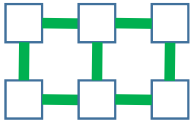


[6] Introduction to High Performance Computing for Scientists and Engineers

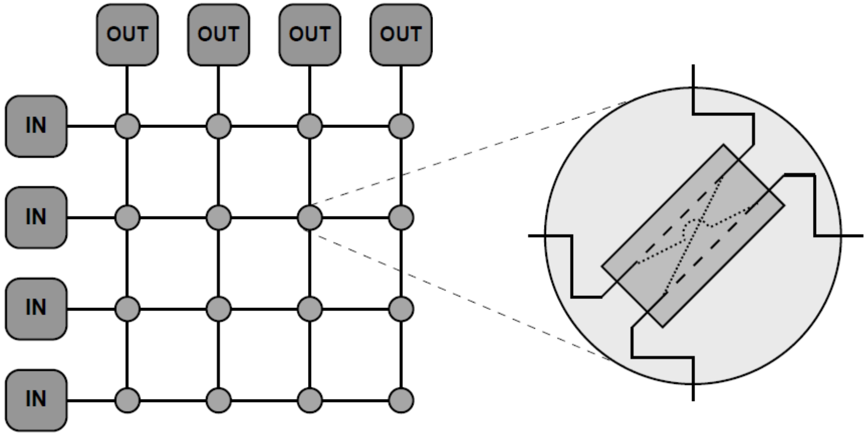
[7] HPC Best Practices @ IO Workshop

Network Building Block 'Switch' inside a HPC system

- A switch is an important network building block inside a HPC system that affects performance
- Think about workers processing data and interacting with each other → switch matters!
- Advanced programming techniques need to take the hardware interconnect into account



- Single fully non-blocking switch
  - All pairs of ports can use their full bandwidth concurrently
  - E.g. 2D cross-bar switch and each circle represents possible connections between two involved IN/OUT devices
  - Aka '2x2 switching element'
  - Aka 'four-port non-blocking switch'

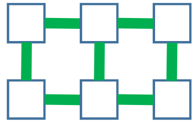


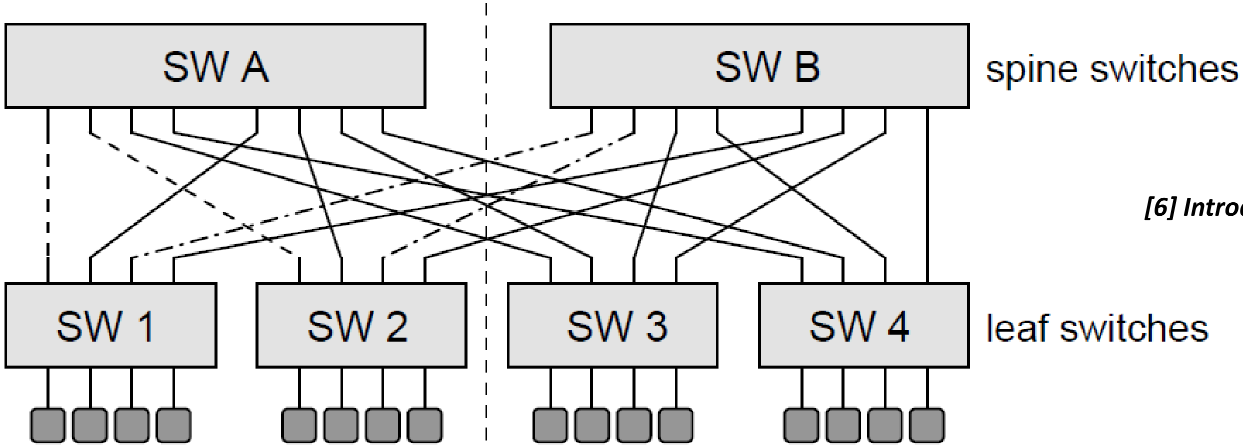
[6] Introduction to High Performance Computing for Scientists and Engineers

- Alternative
  - [partly/completely] single switch with bus design with limited bandwidth

Combining Network Building Blocks as FatTree (1)

- Fully non-blocking full-bandwidth fat-tree network
  - Having two switch layers (leaf and spine)
  - Keeps the 'non-blocking' feature across the whole system via two layers



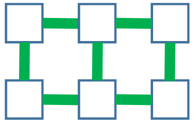


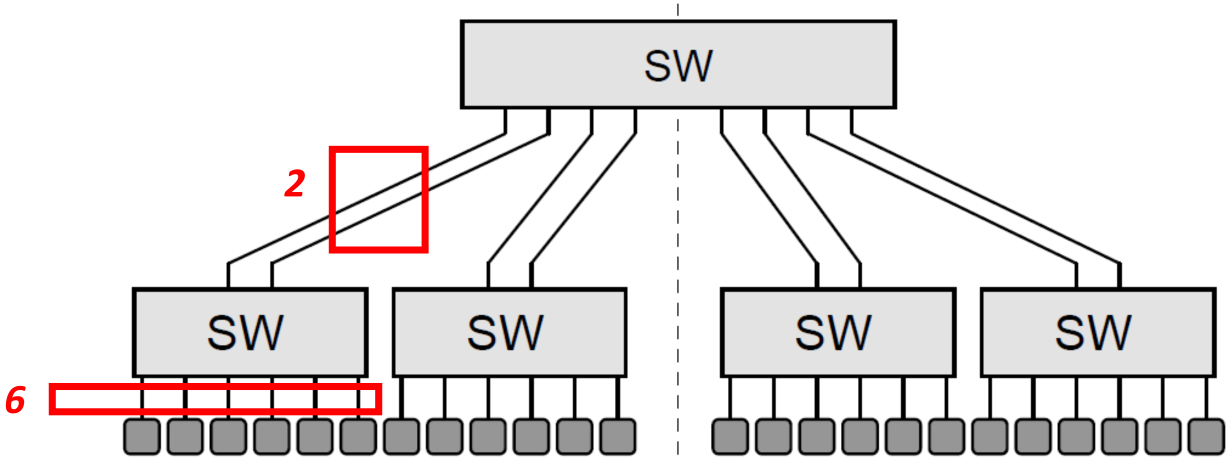
[6] Introduction to High Performance Computing for Scientists and Engineers

- **Here a group of workers processing data 'enjoy' full non-blocking communication**
- **Location of the workers here is not very crucial to the application performance**

Combining Network Building Blocks as FatTree (2)

- Fat-tree network with bottleneck (when # CPUs high)
  - Bottleneck is '1:3 oversubscription' of communication link to spine
  - Only four nonblocking pairs of connections are possible
  - Common in very large systems → safe costs (cable & switch hardware)

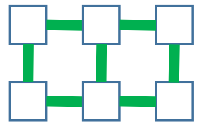




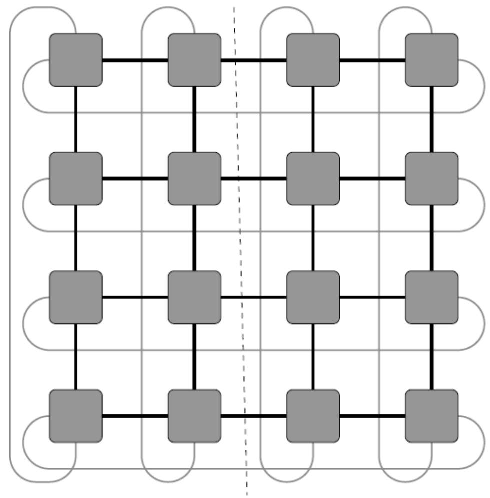
[6] Introduction to High Performance Computing for Scientists and Engineers

- **The location of the workers processing data is crucial for application performance here**

Mesh Networks



- Selected Facts
  - Often in the form of multi-dimensional hypercubes
  - Computing entity is located at each Cartesian grid intersection
  - Idea: connections are wrapped around the boundaries of the hypercube to form a certain torus topology
  - No direct connections between entities that are not next neighbours (but ok!)



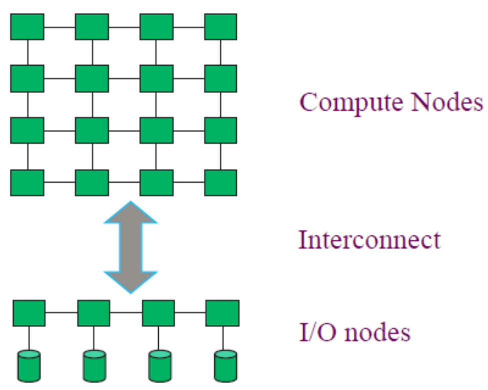
- Example: A 2D torus network
  - Bisection bandwidth scales with $\sqrt{N}$

[6] Introduction to High Performance Computing for Scientists and Engineers

- **Fat-Tree switches have limited scalability in very large systems (price vs. performance)**
- **Bisection bandwidth with scaling in large systems often via mesh networks (e.g. 2D torus)**

Example of Large-scale HPC Machine & I/O Setup

- Example: JUQUEEN
  - IBM BlueGene/Q
- Compute Nodes
  - 28 racks (7 rows à 4 racks)
    28,672 nodes (458,752 cores)
  - Rack: 2 midplanes à
    16 nodeboards (16,384 cores)
  - Nodeboard: 32 compute nodes
  - Node: 16 cores
- Dedicated I/O Nodes
  - 248 (27x8 + 1x32) connected to 2 CISCO Switches



[9] R. Thakur, PRACE Training, Parallel I/O and MPI I/O

[10] JUQUEEN HPC System

- **The I/O node cabling connects the computing nodes via dedicated I/O nodes to storages**

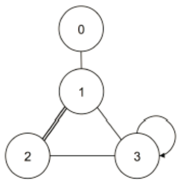
Communication Optimization by Task-Core Mappings (1)

- Approach:
  - Place often-communicating processes on neighboring nodes
  - Requires known communication behavior
  - Measurements via MPI profiling interface

Execution units → processing elements
i.e. processes → i.e. CPUs

- Identification of applicable 'task-core mapping' approach
  - E.g. graph model describes task communication & hardware characteritics
  - Obtain communication characteristics via sourcecode or profiling
  - Obtain hardware characteristics via vendor information (e.g. IBM redbooks)

- **Optimal placement of execution units to processing elements is an NP-hard-problem**
- **n! possibilities to map n execution units to the same number of n processing elements**
- **Topology aware task mapping for I/O patterns exists**



$G_t = (T, E, f)$

$T = \{t_0, t_1, t_2, t_3\}$

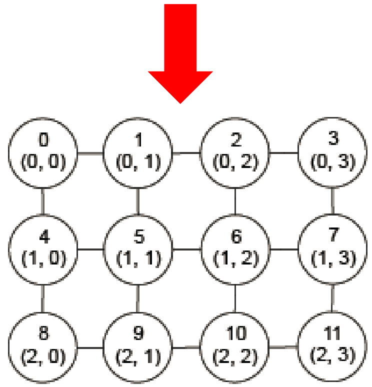
$E = \{\{t_0, t_1\}, \{t_1, t_2\}, \{t_1, t_3\}, \{t_2, t_3\}, \{t_3\}\}$

f:

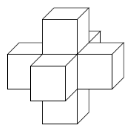
$e \in E_1$	$f_1(e)$
$\{t_0, t_1\}$	1
$\{t_1, t_2\}$	2
$\{t_1, t_3\}$	1
$\{t_2, t_3\}$	1
$\{t_3\}$	1

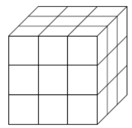
Communication Optimization by Task-Core Mappings (2)

- Application of calculated mappings
  - For regular graphs (tori): Mapping of regular shapes
  - E.g. experiments run on Bluegene/Q JUQUEEN
- Scientific application (cf. Lecture 2)
  - Heatmap as three-dimensional simulation for heat expansion
  - Values of boundary cells are exchanges with neighboring placed ranks
  - Heatmap is divided into equally sized cubes
  - Heat expansion per cube is calculated by a single rank
  - Two different expansion algorithms
  - Using e.g. 'heuristics' for task/core placements



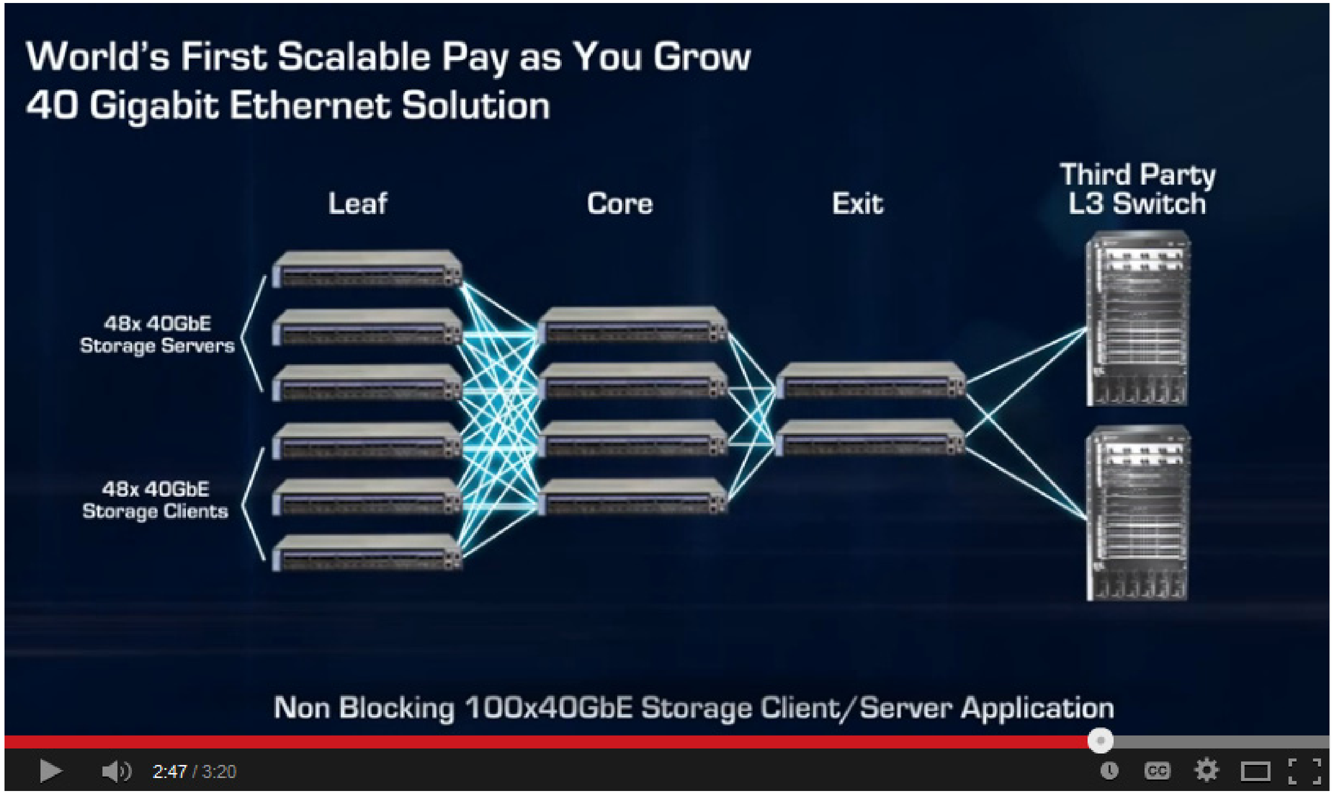
- **Optimized task core mappings enable performance gains between 1-3% (e.g., heatmap application example)**


Expansion 1


Expansion 2

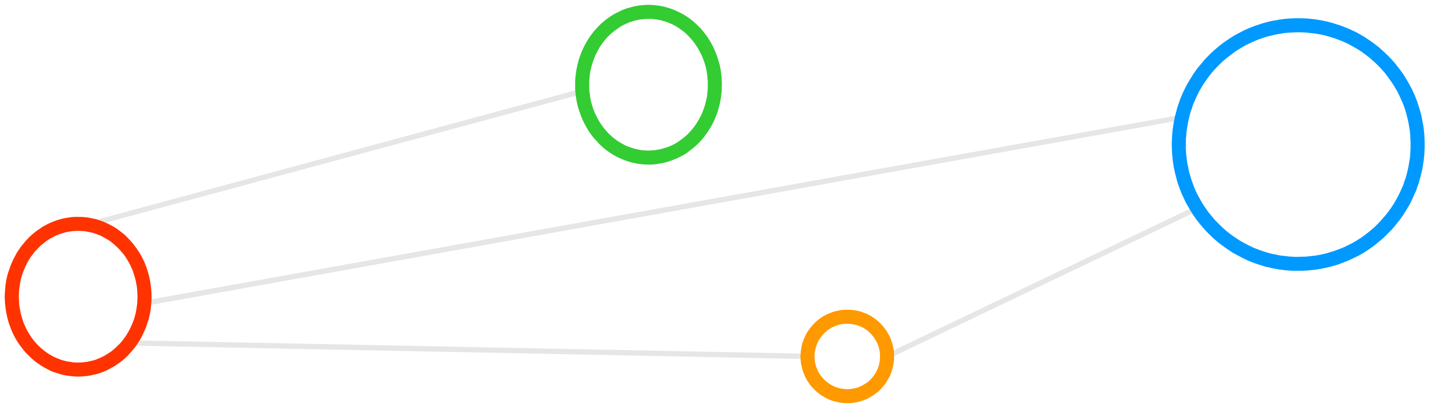
```
for (z = 1; z <= size; z++) {
    for (y = 1; y <= size; y++) {
      for (x = 1; x <= size; x++) {
        new_map[x][y][z] = ( old_map[x][y][z-1]
  + old_map[x][y-1][z] + old_map[x-1][y][z]
  + old_map[x][y][z]  + old_map[x+1][y][z]
  + old_map[x][y+1][z] + old_map[x][y][z+1] ) / 7;
      }
    }
  }
```

[Video] PEPC – Particle Acceleration Application



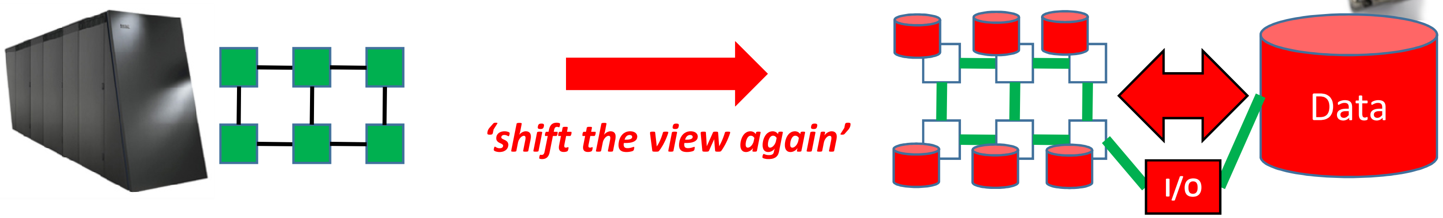
[8] Mellanox YouTube Video

MPI Parallel I/O Techniques



Parallel I/O Techniques – Motivation

- (Parallel) applications that emphasize on the importance of data
  - Not all data-intensive or data-driven applications are 'big data' (volume)
  - HPC simulations of the real world that generates very large volumes of data
- Synthesize new information from data that is maintained in distributed (partly unique) repositories and archives
  - Distributed across different organizations and computers/storages
- Data analysis applications that are 'I/O bound'
  - I/O dominates the overall execution time
  - I/O performance crucial for overall performance



> ➢ **The complementary course Cloud Computing & Big Data – Parallel & Scalable Machine & Deep Learning offers much more techniques**

What means I/O?

- Important (time-sensitive) factors within HPC environments
  - Characteristics of the computational system (e.g. dedicated I/O nodes)
  - Characteristics of the underlying filesystem (e.g. parallel file systems, etc.)

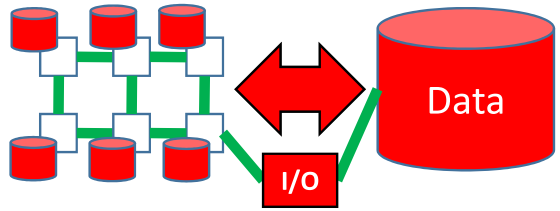
modified from [6] Introduction to High Performance Computing for Scientists and Engineers

- **Input/Output (I/O) stands for data transfer/migration from memory to disk (or vice versa) within a MPI application**

➢ **The course Cloud Computing & Big Data – Parallel & Scalable Machine & Deep Learning offers distributed file system techniques**

I/O Challenges in MPI Applications

- I/O performance bottlenecks in many 'locations in applications'
  - Understanding depends on network & I/O patterns
- During an HPC application run
  - Consider the number of processes performing I/O
  - The number of files read or written by processes
  - Take into account how the files are accessed:
    (a) serial access via one process
    (b) shared access via multiple processes
- Before/After HPC application run
  - How can necessary files be made available/archived (e.g. tertiary storage)
  - E.g. retrieving a high number of small files from tapes takes very long time



- An I/O pattern reflects the way of how a MPI application makes use of I/O (files, processes, etc.) in context of computations

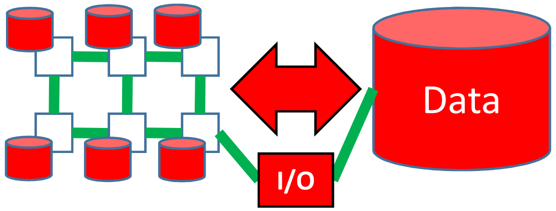
Parallel Filesystems Concept

- File Blocks
  - Distributed across multiple filesystem nodes
  - A single file is thus fully distributed across a ‘disk array’
- Advantages
  - High reading and writing speeds for a single file
  - Reason: ‘Combined bandwidth’ of the many physical drives is high
- Disadvantages:
  - Filesystem is vulnerable to disk failures (e.g. one disk fails → lose file data)
  - Prevent data loss with ‘RAID controllers’ as part of the filesystem nodes
  - Redundant Array of Inexpensive Disks (RAID) levels trade-off vs. data loss

- **A parallel file system is optimized to specifically support concurrent file access**
- **One file that is written to a parallel filesystem is broken up into ‘blocks’ of a configured size (e.g. typically less than 1MB each)**
- **Prevent data loss with Redundant Array of Inexpensive Disks (RAID) levels**

➢ **The course Cloud Computing & Big Data – Parallel & Scalable Machine & Deep Learning offers data storage details (e.g. RAID levels)**

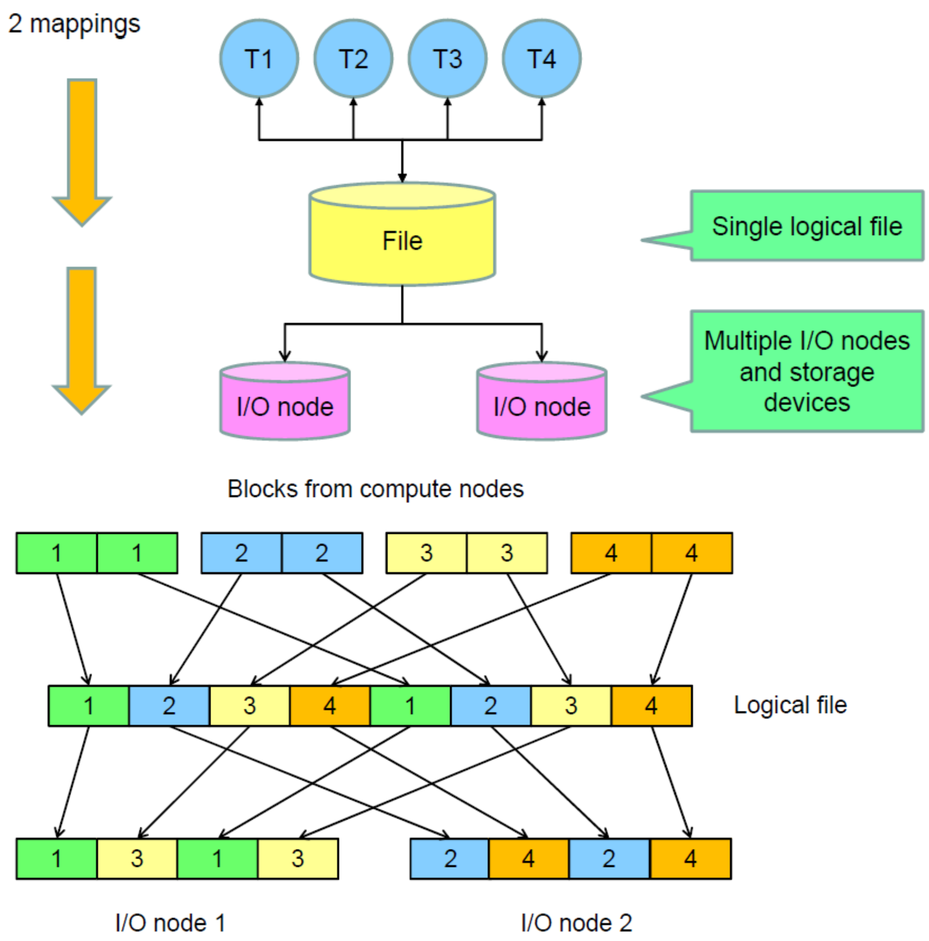
Examples of Parallel File Systems



- General Parallel File System (GPFS) / IBM Spectrum Scale
  - Developed by IBM
  - Available for AIX and Linux
  - Quite expensive solution (but powerful)
  - Moved from HPC-centric computing to 'Big Data' solution (in sales & marketing division)
- Lustre
  - Developed by Cluster File Systems, Inc. (bought by Sun)
  - Movement towards 'OpenLustre'
  - Name is amalgam of 'Linux and clusters'
  - As it is free software it becomes more and more used today
- Parallel Virtual File System (PVFS)
  - Platform for I/O research and production file system for cluster of workstations ('Beowulfs')
  - Developed by Clemson University and Argonne National Laboratory

> - **Widely used parallel file systems are General Parallel File System (GPFS) that is a commercial solution from IBM and Lustre that is open source**
> - **In 2015 IBM rebranded GPFS as IBM Spectrum Scale due to 'Big Data' customers and became a central solution for data-intensive sciences & artificial intelligence**

Concurrent File Access & Two Level Mapping



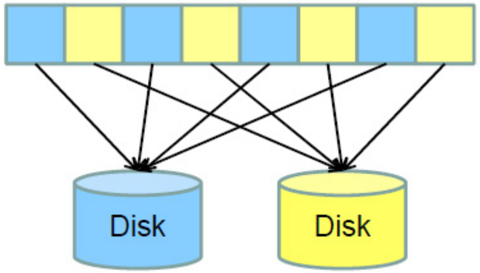
- **Concurrent file access means that multiple processes can access the same file at the same time**
- **Parallel file systems handle concurrent file access via 'single logical files' over multiple I/O nodes**
- **A two Level Mapping means to distribute blocks from compute nodes via logical files (1st level) using underlying multiple I/O nodes (2nd level)**

General Striping Technique

- Striping technique transforms view from a file to flexible ‘blocks‘

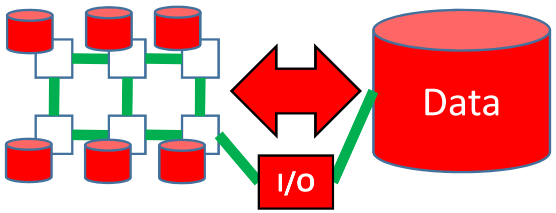
> - **Striping refers to a technique where one file is split into fixed-sized blocks that are written to separate disks in order to facilitate parallel access**

- Striping is a general technique that appears in different contexts
  - Many fields in computer science make use of striping (e.g., data transfer too)
- Two major important factors (to be configured)
  - (e.g. used in MPI I/O ‘hints’ also → later in this lecture)
  - ‘Striping factor’: number of disks
  - ‘Striping unit’: block size
  - Bit-level vs. block-level striping

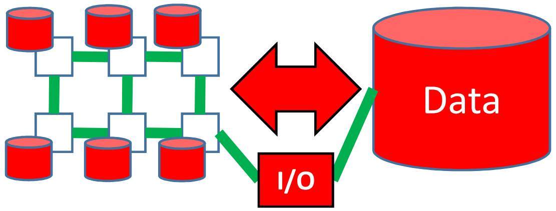


Parallel File Access

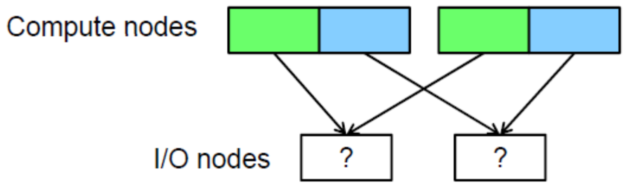
- Comparison with ‘sequential file system’ increases understanding
  - File system translates ‘file name’ into a File Control Block (FCB)
- Parallel File Systems
  - Every ‘I/O node’ manages a subset of the blocks
  - Consequence: Every file has (better: needs) an FCB on every I/O node
- File Access: Two ways to locate FCBs for a file
  - Every I/O node maintains directory structure
  - Central name server: Avoids replication of directory data
- File Creation
  - Filesystem chooses ‘the first’ I/O node (varies)
  - This particular I/O node (‘base node’) will store the first block of the file
  - Specific block is located when first I/O node and ‘striping pattern’ is known
- Question: What about ‘sequential consistency’ when writing?



Sequential Consistency

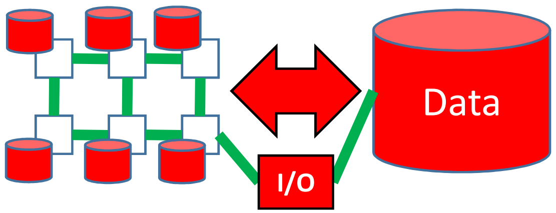


- Two processes on different compute nodes
  - Assumption: Both write to the 'same range of locations in a file'
- 'Sequential consistency'
  - Requires that all I/O nodes write their portions in the same order
  - Write request should appear to occur in well-defined sequence
  - But hard to enforce – I/O nodes may act independently



- Selected Possible Solutions
  - Locking entire files - Prevents parallel access (not an option)
  - Relaxed consistency semantics – application developer is responsible
  - Locking file partitions – prevents access to certain file partitions

File Pointers

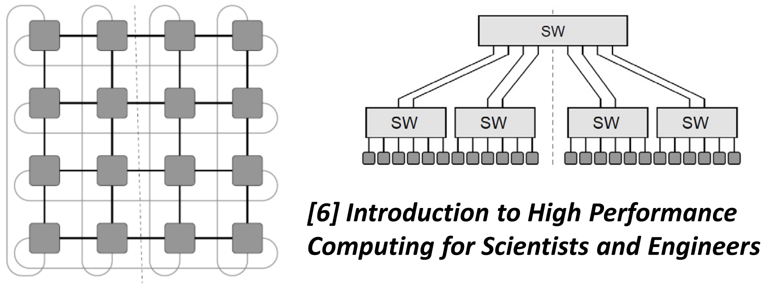


- MPI Applications
  - Need to be aware of 'which processes use which parts of the file'
  - May require processes to skip file sections 'owned by others'
- Shared File Pointers
  - Common in shared-memory programs
  - Inefficient – serializes requests (update file pointer before completing request, 'eager update')
  - Inconsistencies if seek and write operations are separated
- Improvements of Usage
  - Better use 'separate file pointers' or atomic seek & write
  - In UNIX `pread()` and `pwrite()` allow specification of 'explicit offset'

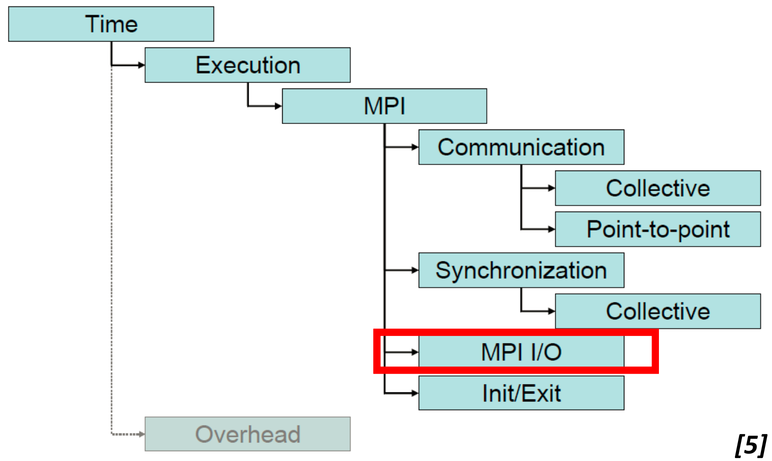
```
Thread 1:                      Thread 2:
seek(location = 100);          seek(location = 200);
write(..., length = 50);       write(..., length = 150);
```

Optimization & Dependencies on Hardware & I/O – Revisited

- Optimizations in terms of software & hardware are important
  - Optimization can be interpreted as using ‘dedicated‘ hardware features (if available)
  - E.g. network interconnections enable different used ‘network topologies‘ (varies in different systems)
  - E.g. parallel codes are tuned applying parallel I/O with parallel filesystems (if parallel filesystem exists)



[6] Introduction to High Performance Computing for Scientists and Engineers

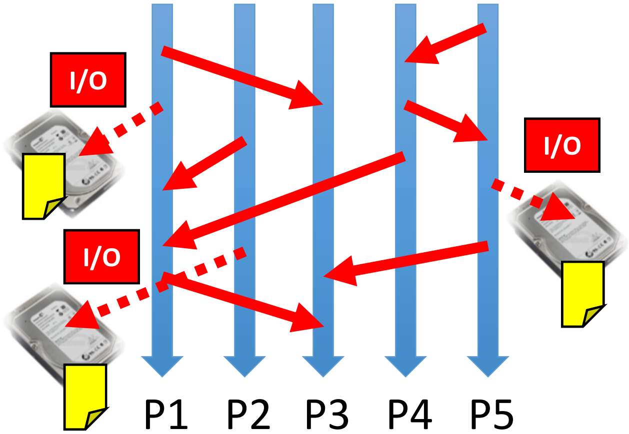


[5] Metrics tour

> **Lecture 9 on debugging, profiling & performance toolsets offers insights into performance analysis tools to understand MPI code better**

MPI I/O

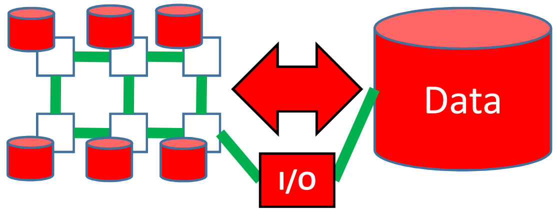
- Different operation modes
  - 'Blocking mode' to finish data operations, then continue computations
  - 'Non-blocking mode' (aka asynchronously) to perform computations while a file is being read or written in the background (typically more difficult to use)
- Supports the concept of 'collective operations'
  - Processes can access files each on its own or all together at the same time
- Provides advanced concepts
  - E.g., file views & data types/structures

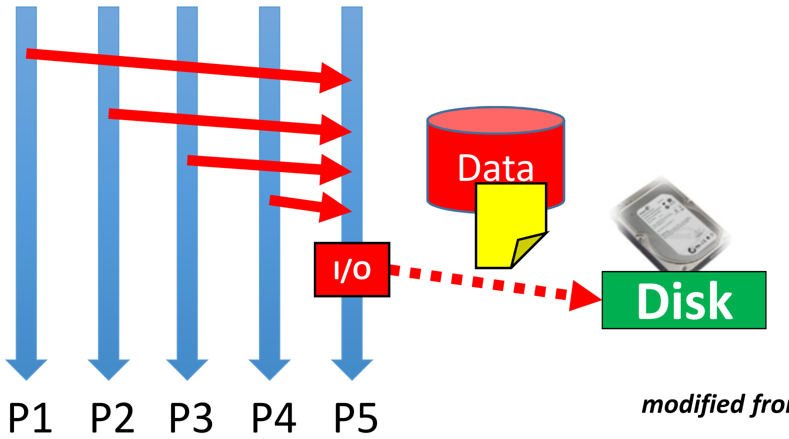


- **MPI I/O provides 'parallel I/O' support for parallel MPI applications**
- **Writing/Receiving files is similar to send/receive MPI messages, but to disk**

Serial I/O: One Process on behalf of Many Processes

- Only one process performs I/O on behalf of all other processors
  - Data aggregation or duplication
  - Limited by single I/O process (e.g. determined by rank as writer role)
- No scalability for (big) data-intensive computing
  - Time increases linearly with amount of (big) data
  - Time increases with number of processes of the parallel application



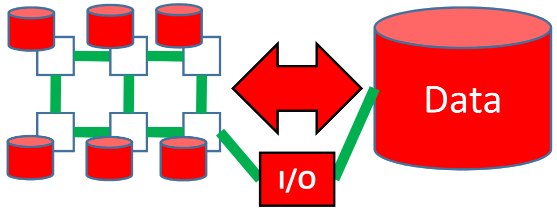


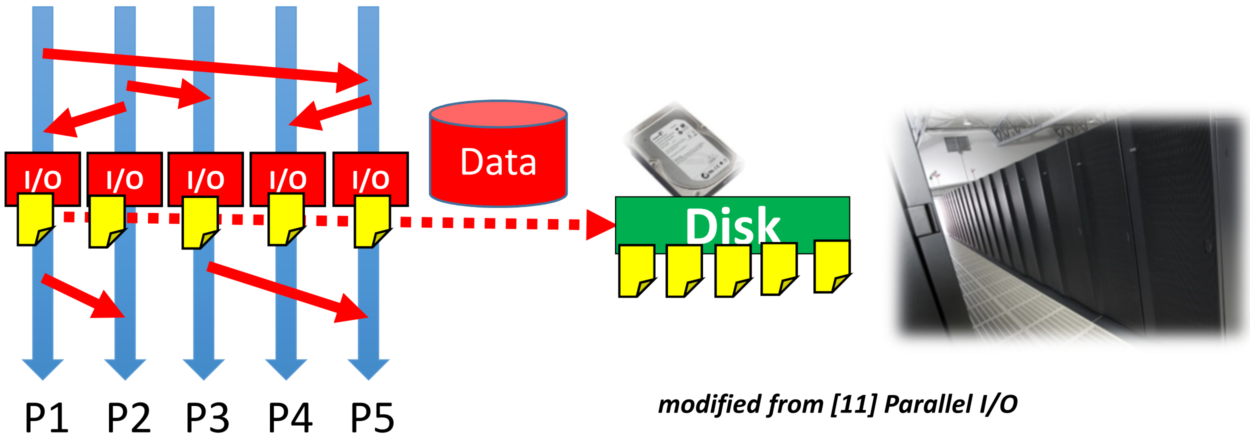
modified from [11] Parallel I/O

- Serial I/O: One process on behalf of many means that one process takes care of all I/O tasks
- Serial I/O increases communication and is slow as well as including load imbalance risks

Parallel I/O: One file per Process

- All processors perform I/O to individual files
  - Limited by file system capabilities
- No scalability for large number of processors
  - Number of files creates bottleneck with metadata operations
  - Number of simultaneous disk accesses creates 'contention' for file system resources
  - E.g., the disk cannot keep up with file I/O requests



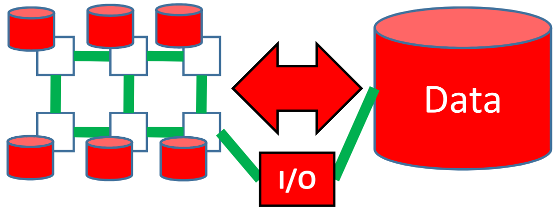


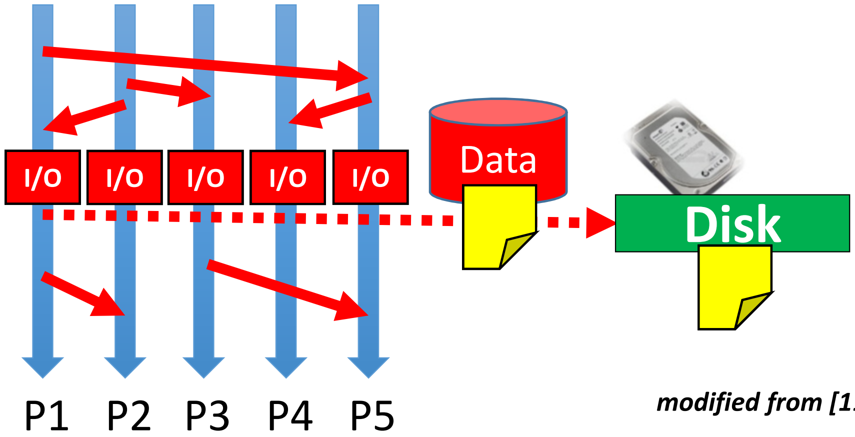
modified from [11] Parallel I/O

- **Parallel I/O: One file per process means that each process takes care of local I/O tasks alone**
- **Parallel I/O is good for scratch but not for output files in applications despite I/O balance**

Parallel I/O: Shared File

- Each process performs I/O to a single file
  - The file access is ‘shared’ across all processors involved
  - E.g. MPI/IO functions represent ‘collective operations‘
- Scalability and Performance
  - ‘Data layout’ within the shared file is crucial to the performance
  - High number of processors can still create ‘contention’ for file systems





modified from [11] Parallel I/O

- Parallel I/O: shared file means that processes can access their ‘own portion’ of a single file
- Parallel I/O with a shared file like MPI/IO is a scalable and even standardized solution

Collective MPI-I/O: Writing integers to a file example

```
#include <stdio.h>
#include <mpi.h>

int main (int argc, char** argv) {
  int rank, size;

  MPI_File fh;
  MPI_Info info;

  char *file_name = "outputfile";

  int buf[10];

  MPI_Init(&argc, &argv);

  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  printf("Hello World, I am %d of %d\n", rank, size);

  MPI_Info_create(&info);

  int rc = MPI_File_open( MPI_COMM_WORLD, file_name,
                          MPI_MODE_CREATE | MPI_MODE_RDWR,
                          info, &fh);
  buf[0] = rank;

  // MPI_File_write_ordered(fh, buf, 1, MPI_INT, &status);
  MPI_File_write(fh, buf, 1, MPI_INT, &status);

  rc = MPI_File_close(&fh);

  MPI_Finalize();
  return 0;
}
```

- A MPI_File represents a file handler that reprents the file and process group of a communicator
- A MPI_Info represents a list of key/value pairs used for providing information to MPI-I/O

- Specifying a file_name that should be opened (or even be created) – but attention: The format is highly implementation dependent

- MPI_Info_create creates an MPI_Info object to be used to provide information to MPI-I/O

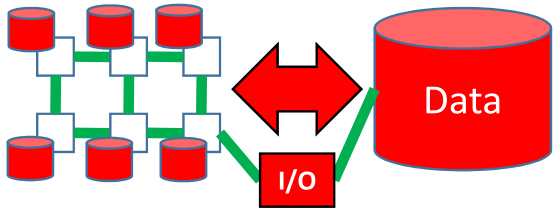
- MPI_File_open opens a specific file collectively across all specified processes being part of the used communicator and sets a file handle

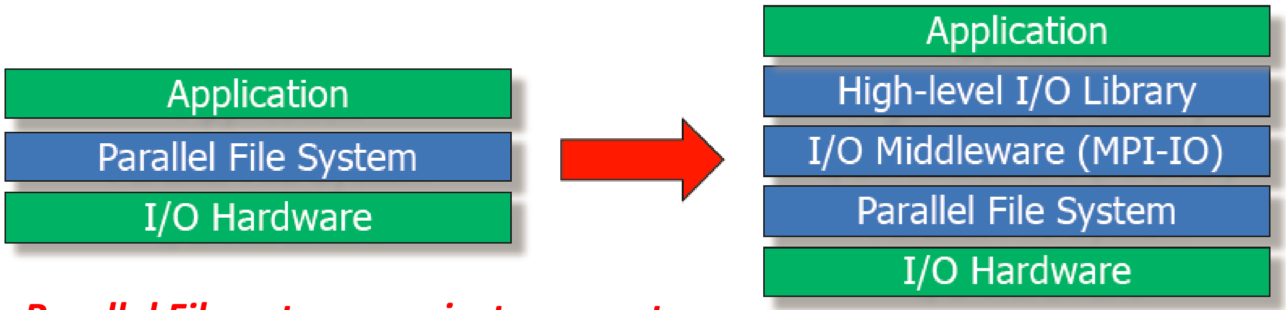
- Requires a buffer (here integer array) of a certain size (e.g. buf[10])
- Requires values for the buffer: here the rank of each MPI process that might be used as identification for further values following in the next parts of the corresponding file is used
- MPI_File_write or related versions write the <u>binary output</u> to the file
- Different between MPI_File_write() and MPI_File_write_ordered() is that the out is not ordered according to ranks or ordered by ranks

- MPI_File_close closes a specific file identified via a certain file handle

MPI I/O & Parallel Filesystems

- Understanding and tuning parallel I/O is needed with 'big data'
  - Leverage aggregate communication and I/O bandwidth of client machines
- Support: Add additional software components/libraries layers
  - Coordination of file access & mapping of application model to I/O model
  - Components and libraries get increasingly specialized / layer
  - High-Level I/O libraries like NetCDF or Hierarchical Data Format (HDF) are standards in the community



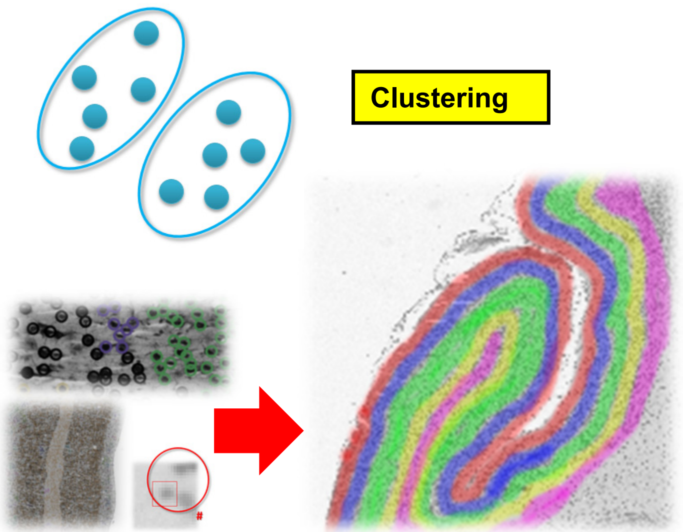


Parallel Filesystems are just one part out of three in the whole I/O process

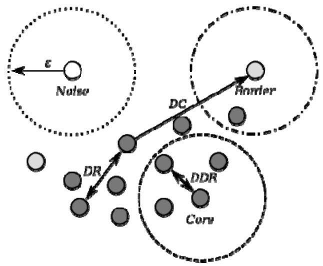
[9] R. Thakur, PRACE Training, Parallel I/O and MPI I/O

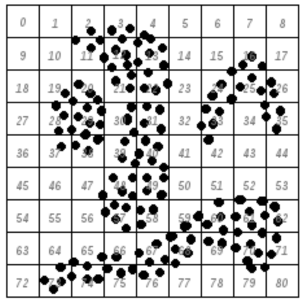
➢ **Lecture 5 offers more details on using Parallel I/O and portable data formats in various simulation sciences & data science applications**

Data Science Example: Using High-Level I/O Hierarchical Data Format (HDF)

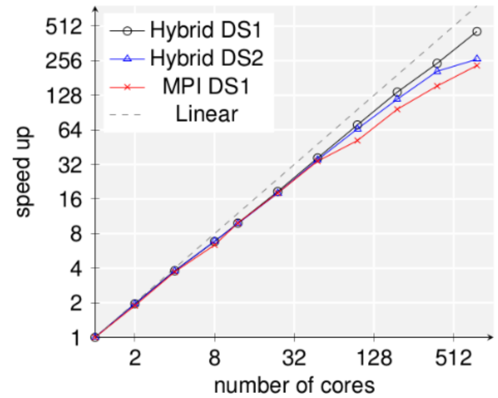


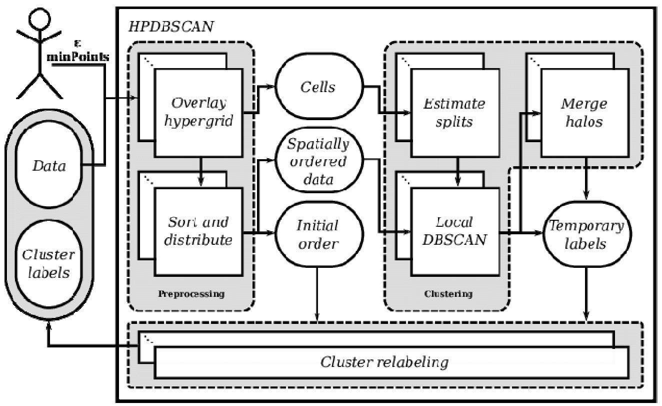
[13] M. Goetz and M. Riedel et al,
Proceedings IEEE Supercomputing Conference, 2015

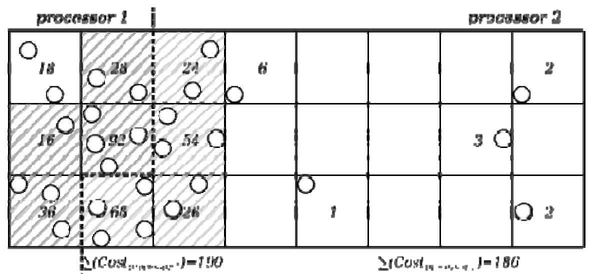




Overlayed spatial grid

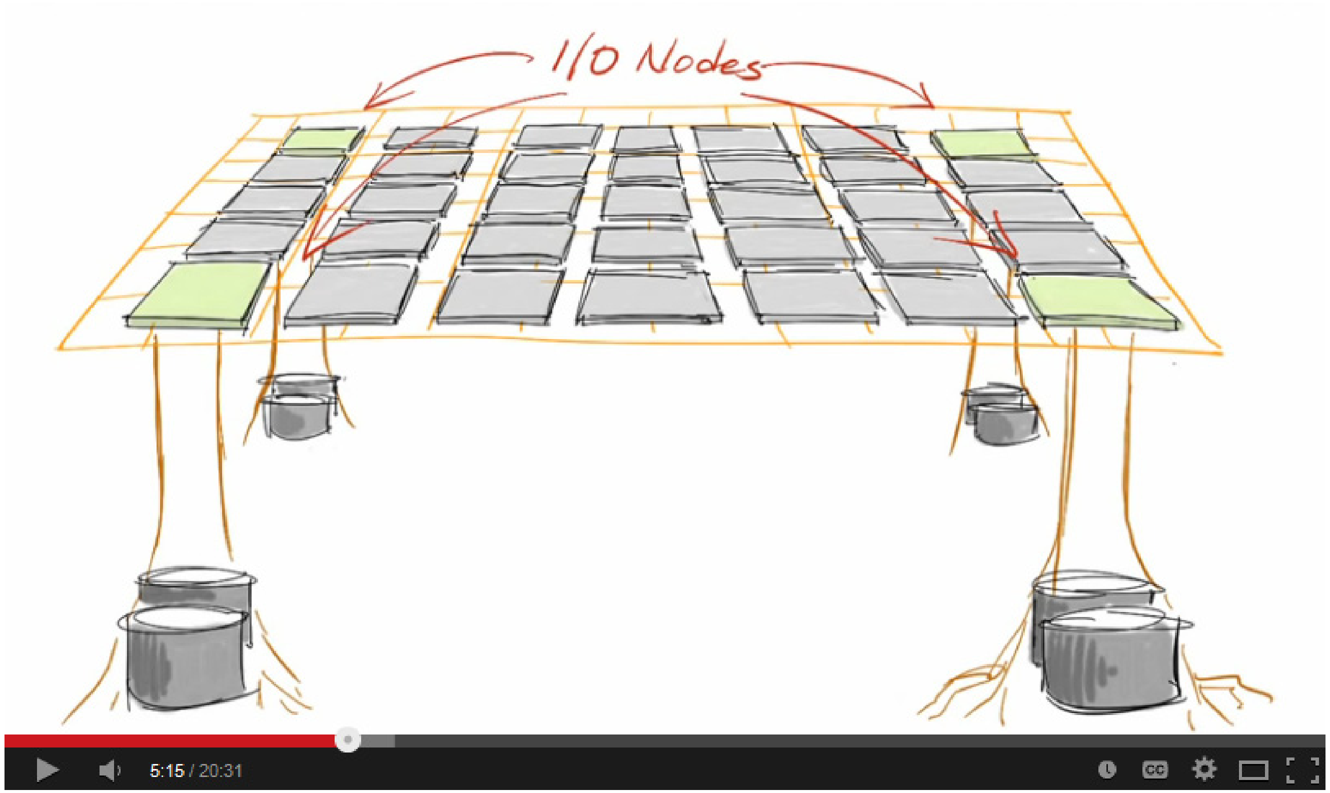






- Lecture 5 offers more details on using Parallel I/O and portable data formats in various simulation sciences & data science applications

[Video] Parallel I/O with I/O Nodes



[12] YouTube Video, 'Simplifying HPC Architectures'

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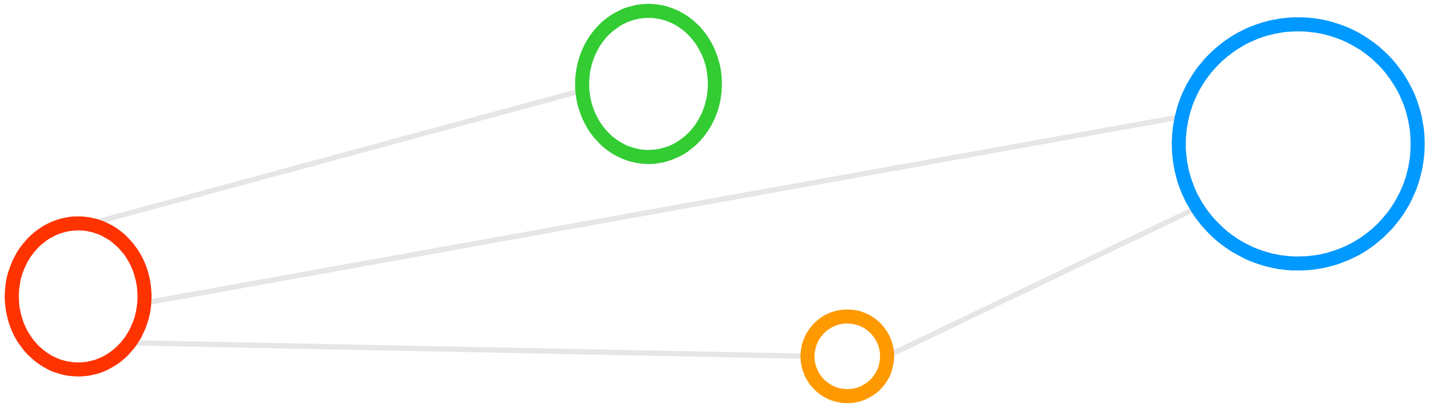

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